

The Effect of Operating Parameters on Soot Emissions in GDI Engines

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ABSTRACT

Due to the upcoming regulations for particulate matter (PM) emissions from GDI engines, a computational fluid dynamic (CFD) modeling study to predict soot emissions (both mass and solid particle number) from gasoline direct injection (GDI) engines was undertaken to provide insights on how and why soot emissions are formed from GDI engines. In this way, better methods may be developed to control or reduce PM emissions from GDI engines. In this paper, the influence of engine operating parameters was examined for a side-mounted fuel injector configuration in a direct-injection spark-ignition (DISI) engine. The present models are able to reasonably predict the influences of the variables of interest compared to available experimental data or literature. For a late injection strategy, effects of the fuel composition, and spray cone angle were investigated with a single-hole injector. For an early injection strategy, the effects of multi-component fuel surrogates for gasoline, SOI timings and wall temperatures were studied with a six-hole injector. The investigations confirmed the necessity to consider the multi-component fuel composition and also demonstrate how and why wall films significantly contribute to soot emissions from DISI engines.

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INTRODUCTION

The percentage of gasoline vehicles with DISI engines is expected to continue increasing significantly with a projection of 60% of all new vehicles by 2016 in the United States[1]. However, more stringent regulations for DISI engines have also been proposed recently, and the number-based regulation has become a new challenge for DISI engines, which historically only needed to meet a mass-based regulation. Therefore, DISI engines are still under scrutiny because of the particulate or smoke emissions they can produce.

Particulate matter emission from internal combustion engines usually can be divided into solid (ash, carbon) and volatile components (liquid phase). The solid particles mainly consist of agglomerated carbonaceous primary particles, which are usually described as soot, and are usually formed during combustion in locally rich regions. Both organic compounds (i.e., unburnt hydrocarbons and oxygenated hydrocarbons) and inorganic compounds (i.e., sulfur dioxide, nitrogen dioxide, and sulfuric acid) can be absorbed upon those solid particles [2, 3, 4, 5]. A small fraction of the fuel and some atomized and evaporated lube oil can escape oxidation and also appear as volatiles in the exhaust. The formation of volatile nanoparticles strongly depends on the dilution rate, temperature, the cooling process of the exhaust, residence times, surface area of pre-existing particles, and humidity [6, 7, 8]. The composition of the exhaust particles also strongly depends upon where and how they are collected. For instance, nucleation, condensation and adsorption transform volatile components to solid and liquid PM as the exhaust is diluted and cooled, while most of the volatile materials are in the gas phase in the tailpipe, where temperatures are high enough.

Therefore, only the carbonaceous portion of engine particulate emissions is modeled in this work (i. e., smoke, dry particulate, or elemental carbon (EC)).

For gasoline fuel the light-end components tend to play significant roles in the spray, ignition and combustion processes, while the heavy-end components vaporize later, and exert important roles in soot emissions, especially in the presence of wall films [9, 10, 11]. The aromatic structure of toluene addition was likely to be responsible for higher soot emissions in Ref.[12]. The influence of multi-component fuel surrogates for both fuel physical properties and chemistry reactions will be investigated in this work.

For a prototype DI engine with a side-mounted injector, a strong correlation between smoke emissions and spray cone angle has been observed that has been directly attributed to variations in the fuel film thickness on the piston[13]. Similar experimental observations have also been presented from parametric studies of the effect of spray cone angle on soot emissions for a GDI combustion system with a side-mounted injector[14]. The smoke amount reduces with increased the spray cone angle due to less spray impingement on the piston cavity. In a DISI optical engine with a stratified-charge combustion system, the liquid fuel is concentrated inside the bowl in the region opposite the injector side, and carbon deposits have been observed by Han et al.[15] to build up inside the piston bowl due to the rich mixture burning near the liquid fuel film regions. A decrease of wall films was predicted with a wider spray cone angle, in agreement with the decreased smoke in the experiments.



Injection timing is also known to be important since it influences the amount of fuel-wall impingement, and optimization of injection timing is necessary to avoid spray over-penetration and the associated unintended wetting of chamber surfaces [11, 16, 17, 18, 19, 20]. The influence of injection timing on fuel wall wetting for a combustion system with an intake-side-mounted injector was also seen in CFD modeling works [21, 22]. Injection timing is also a key factor for soot emissions. Yang et al.[23] reported that retarding the injection timing led to more stable combustion for an overall lean air/fuel mixture due to enhanced local charge stratification. However, extreme retardation of the injection timing resulted in a significant increase of smoke emissions, indicated by a sharp increase of the AVL filter smoke number (FSN). Moreover, the injection timing is also influenced by the in-cylinder pressure, which influences spray atomization. A correlation of the measured smoke emissions with the amount of calculated fuel wall wetting and the wall film thickness is also observed in CFD modeling for a range of injection timings in engine tests[21]. The correlation suggests that a small amount of fuel impinging on the piston crown can produce a considerable amount of smoke if the resultant wall film is relatively thick. The temperature of wall surfaces is also found to have a significant effect on film vaporization. Generally, slow wall film vaporization is observed for a cold wall, leading to degraded spatial uniformity of the fuel-air mixture, while enhanced wall film vaporization exhibits when the surface temperature ranges from 90 °C to 130 °C. Recent experiments[24] report that a seemingly small change of wall temperature causes a significant change of heat flux, leading to the changes in the fuel depositing on the surfaces.

The objective of this work was to investigate the influence of fuel composition, spray cone angle, injection timing, and wall temperature for early- and late-injection strategies on soot emissions in a DISI engine using a newly formulated version of the KIVA CFD code[25], which can predict in-cylinder distributions of spray, wall films, spark-ignition and soot emissions (both mass and solid particle number) to provide insight on how and why soot emissions are formed from GDI engines. In this way, better methods may be developed to control or reduce PM emissions from GDI engines

CFD MODEL

The multi-dimensional KIVA3V Release 2 code, coupled with a list of improved submodels (see [Table 1](#)), was used in this work. The model was formulated to predict soot emissions (mass and solid particle number) using multi-component fuel surrogates to represent gasoline in full-cylinder DISI engines. The performance of the models in predicting particle size distributions is investigated for an SI engine at premixed operating conditions[26].

Table 1. Submodels in KIVA.

Models	Model description
Fuel break-up model	KH break-up model for primary break-up of injected spray parcels and RT breakup model for secondary break-up [27].
Gasjet model	Reduce grid-dependence of near-nozzle droplet-gas momentum exchange [28].
Droplet collision model	O'Rourke droplet collision model [29], further improved by the radius-of-influence method [28].
Droplet vaporization model	A discrete multi-component fuel vaporization model [30].
Turbulence model	k-ε RNG method [31], further improved with the G-RNG model [32].
Spray/wall interaction model	Spray/wall interaction model of O'Rourke et al. (OA model) [33, 34], further improved in Ref. [25] to reduce grid dependence of film vaporization.
Semi-detailed soot model	A semi-detailed soot model [35], which is coupled with PAH chemistry reactions, further improved in Ref. [26].
Spark ignition model	Discrete Particle Ignition Kernel (DPIK) spark ignition model [36].
G-equation flame propagation model	A level set method (G-equation) implemented by Refs. [37, 38].
Chemistry Solver	A Jacobian Chemistry solver: SpeedCHEM [39].
Chemistry mechanism	n-heptane/iso-octane/toluene/PAH mechanism in Ref. [40], further improved to consider toluene pyrolysis reactions in Ref. [25].

MODEL APPLICATION

Geometry and Operating Conditions of a DISI Engine

The engine's geometric specifications are given in [Table 2](#). The computational mesh contains around 79,000 cells, including the intake and exhaust manifolds and the cylinder, as shown in [Figure 1](#). The computations were usually started near intake TDC and terminated at 80 ° after compression TDC. Therefore, intake, compression, fuel injection, spark ignition and combustion processes were simulated.

Table 2. DISI Engine Specifications.

Dimension	Unit	Value
Compression ratio	(-)	12.0: 1
Bore	(mm)	89.0
Stroke	(mm)	79.5
Cylinder head	(-)	Pent-roof
Piston shape	(-)	Bowl-in-piston
DI injector	(-)	Side-mounted
Valves	(-)	2 intake/2 exhaust
IVO/IVC	(°ATDC)	-400/-88
EVO/EVC	(°ATDC)	-578/-278

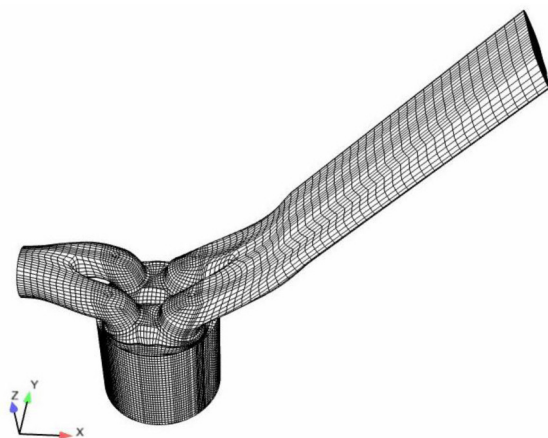


Figure 1. Computational mesh of the spark-ignition direct-injection engine with pent-roof and bowl in piston, 79,000 cells at BDC including intake and exhaust valves.

Table 3. DISI engine specification of late injection strategy.

SOI ($^{\circ}$ ATDC)	-75
EOI ($^{\circ}$ ATDC)	-68
Injection mass (mg/cycle)	6.88
Spray cone angle (degree)	10
Spark timing ($^{\circ}$ ATDC)	-33
Fuel (baseline)	iso-octane
A/F ratio	51.6
Engine speed (rev/min)	1500.0

Table 4. DISI engine specifications of early injection strategy

	Unit	Experiment [41] (for reference)	Simulation
Bore	(mm)	92.5	89
Stroke	(mm)	86.7	79.5
Compression ratio	(-)	10:1	12:1
Speed	(rev/min)	1250	1250
Piston	(-)	Bowl-in-piston	Bowl-in-piston
Injection pressure	(bar)	100	100
Injection timing	($^{\circ}$ ATDC)	-330/-320/-290	-330/-320/-290
FSN	(-)	2.62/1.62/0.05	
Fuel	(-)	91 RON gasoline	91 RON gasoline surrogates
Fuel injector	(-)	Side-mounted 6-hole	Side-mounted 6-hole
Global equivalence ratio	(-)	1.0	1.0

In the following sections the influence of fuel compositions, spray cone angle will be investigated using the late injection strategy, while the influence of wall temperature and start of injection (SOI) timing were studied for early injection operating conditions. Table 3 illustrates the operating conditions for late injection study, and the early injection operating conditions are presented in Table 4.

Fuel Modeling

As introduced in Table 1, the current CFD code uses a discrete multi-component approach to model the physical properties of the fuel components. This approach has been successfully applied to diesel and gasoline engines and represents great advantages in modeling the characteristics of real transportation fuels [30, 42, 43, 44, 45].

The optimum physical compositions for real transportation fuels were obtained by a novel methodology based on local optimization and sensitivity analysis in terms of matching the distillation curve, mass fraction of family groups (saturates, aromatics and olefins), hydrogen to carbon (H/C) ratio, Cetane Number (CN) and the Research Octane Number (RON)[44]. The surrogates are introduced as ‘fuel physical surrogates’.

However, reaction chemistry mechanisms are not available for all the individual components proposed in modeling the fuel physical surrogates. Therefore the group chemistry representation (GCR) approach proposed by Ra and Reitz[42] was utilized to represent the fuels chemical reactions. These surrogates are ‘fuel chemical surrogates’, which are used to model fuel oxidation processes. The fuel physical surrogates are grouped based on their chemical classes and the combustion characteristics of each group are represented by representative chemical surrogates, which do have available fuel chemistry mechanisms.

In this work, the chemical classes were classified into groups based on their molecular structure: viz., n-paraffins, iso-paraffins and aromatics. They are therefore represented using available chemical mechanisms for n-heptane, iso-octane and toluene, respectively, as suggested by Ra and Reitz[42].

Table 5 presents the proposed fuel physical surrogates and the corresponding fuel chemical surrogates for 91 RON gasoline. The fuel physical surrogates were found to represent experimental fuel distillation curve reasonably well, and it is of great importance to model the boiling range of the fuel to be able to predict its vaporization characteristics for engine applications. The simulated distillation curve of the fuel surrogates was compared with the experimental distillation curve of 91 RON gasoline, as shown in Figure 2, although minor discrepancies still exist for the heavy-end and light-end of the distillation curve, the current 10-component fuel surrogate was considered to be satisfactory for the present study.

Table 5. Experiment and modeling surrogates for 91 RON gasoline [41].

Experiment		Simulation					
		Physical surrogates					Chemical surrogates
	Mass fraction (%)	Component name		Molecular weight (g/mol)	Boiling temperature (K) at 1 bar	Mass fraction (-)	
Saturates	70.3	n-heptane	n-C7H16	100	371.6	0.05921	n-heptane
		n-decane	n-C10H22	142	447.2	0.06023	
		2,2,3,3 tetramethylhexane	C10H22	142	413.5	0.02935	iso-octane
		iso-pentane	i-C5H12	72	301.2	0.31702	
		iso-heptane	i-C7H16	100	363.2	0.13954	
		iso-octane	i-C8H18	114	372.5	0.09062	
Aromatics (Olefins)	26.4 (3.3)	toluene	C7H8	92	383.8	0.09932	toluene
		m-xylene	C8H10	106	412.2	0.07041	
		m-cymene	C10H14	134	448.2	0.10484	
		l-hexene	C6H12	84	336.2	0.02888	

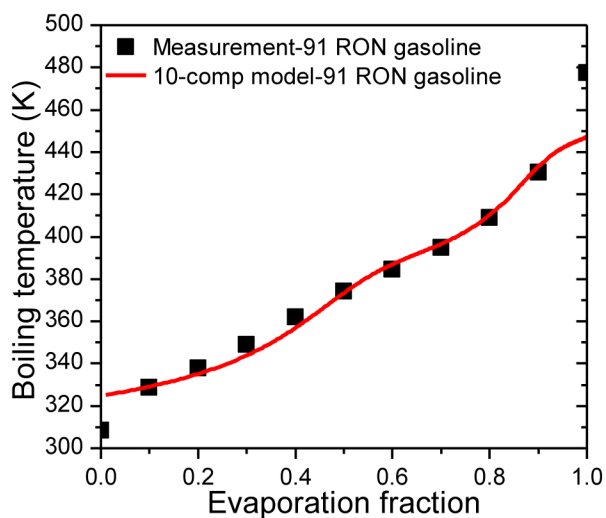


Figure 2. Measured and predicted distillation curves of a gasoline fuel (91RON). Experimental distillation curves from Ref.[41].

Fuel Composition

The fuel composition investigated is represented in Table 6, where case 1 used only iso-octane as the fuel surrogate, as has been done in earlier studies [25, 46]. For cases 2 and 3, 30% of the iso-octane mass fraction is substituted by two aromatics with different boiling

temperatures (i.e., toluene and m-cymene), respectively, which are correspondingly used as the fuel physical surrogates, while toluene is used as the chemical surrogate for both toluene and m-cymene, as shown in Table 5.

The predicted mass of fuel film on the different wall surfaces is shown in Figure 3 for the three cases at the start of ignition and at 80 °ATDC, respectively. As can be seen, the mass of total wall films from case 3 is approximately 3 times from case 1, and the film mass from case 2 is almost twice that of case 1. This is mainly due to the different boiling temperatures of iso-octane, toluene and m-cymene, as seen in Table 5. By 80 °ATDC, no films are left for case 1, while the highest film mass is observed for case 3.

Table 6. Fuel compositions investigated in late-injection DISI engine.

Case #	Fuel compositions	Physical surrogates	Chemical surrogate
Case 1 (baseline case)	iso-octane	iso-octane	iso-octane
Case 2	0.7 iso-octane/ 0.3 toluene	iso-octane/ toluene	iso-octane/ toluene
Case 3	0.7 iso-octane/ 0.3 m-cymene	iso-octane/ m-cymene	iso-octane/ toluene